First-Principles Study of Electromigration in the Metallic Liquid State of the GeTe and Sb_2Te_3 Phase Change Compounds

Supporting Information

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TABLE S1: Primitive vectors (Å) of the 64-atom supercell of liquid GeTe.

	x	y	z
a	8.6085	0.0000	0.0000
b	-4.3043	7.4552	0.0000
c	0.0000	0.0000	29.7679

TABLE S2: Primitive vectors (Å) of the 65-atom supercell of liquid Sb_2Te_3.

	x	y	z
a	8.6085	0.0000	0.0000
b	-4.3043	7.4552	0.0000
c	0.0000	0.0000	36.0429

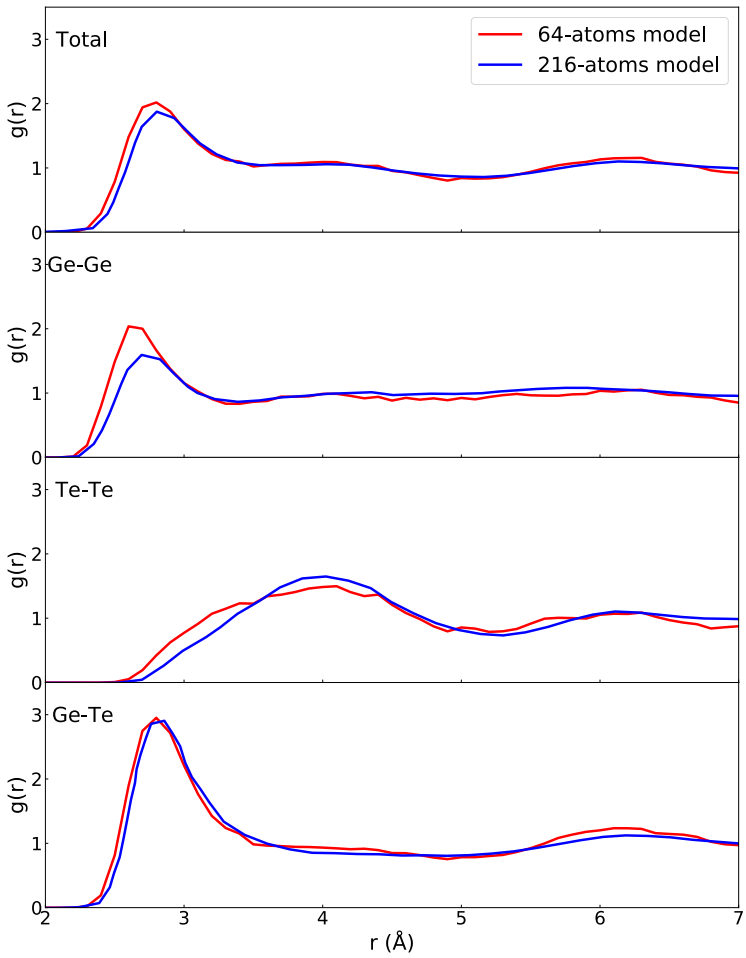

FIG. S1: Total and partial pair correlation functions of GeTe in the 64-atom prismatic cell (see Table S1) at 1020 K compared with the result from a 216-atom cubic cell at 1150 K from Ref. (1).

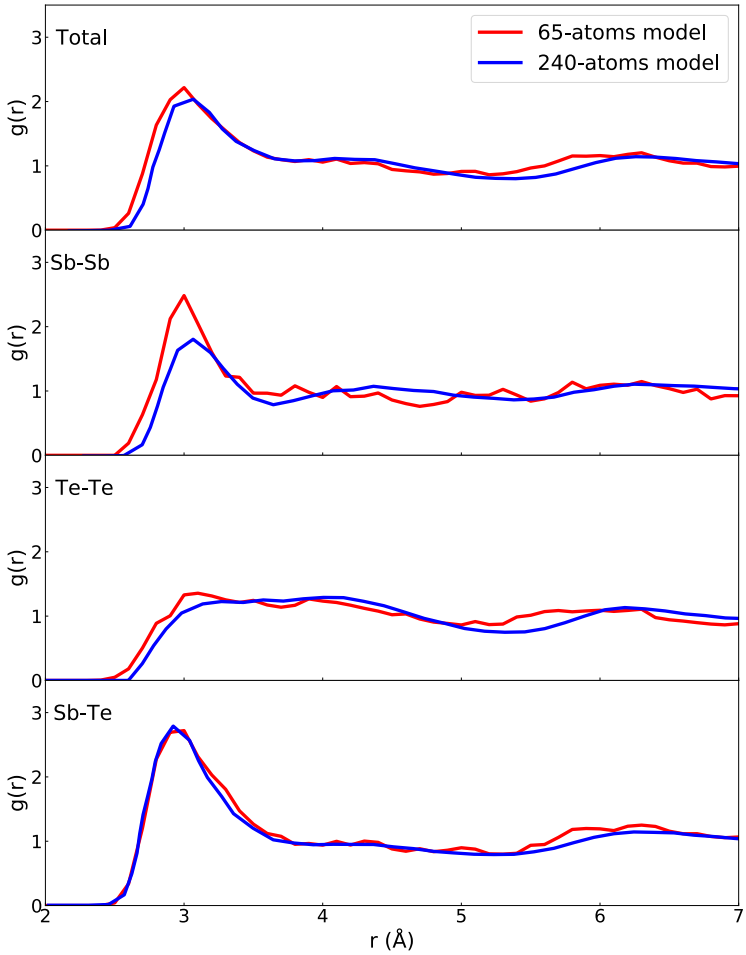

FIG. S2: Total and partial pair correlation functions of Sb_2Te_3 in the 65-atom prismatic cell (see Table S2) at 920 K compared with the result from a 240-atom cubic cell at 1003 K from Ref. (2) .

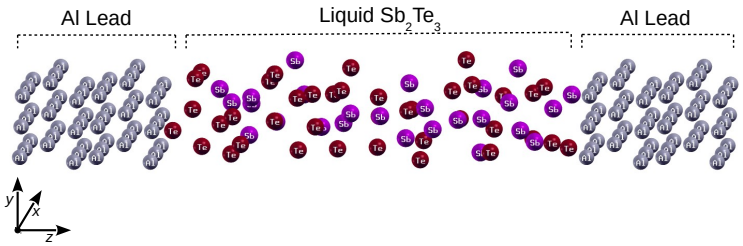

FIG. S3: Atomic model of the Al/Sb_2Te_3/Al junction used for the NEGF+DFT calculations. The model consists of 65 atoms of Sb_2Te_3 (13 formula units) and 108 atoms of Al in the two electrodes.

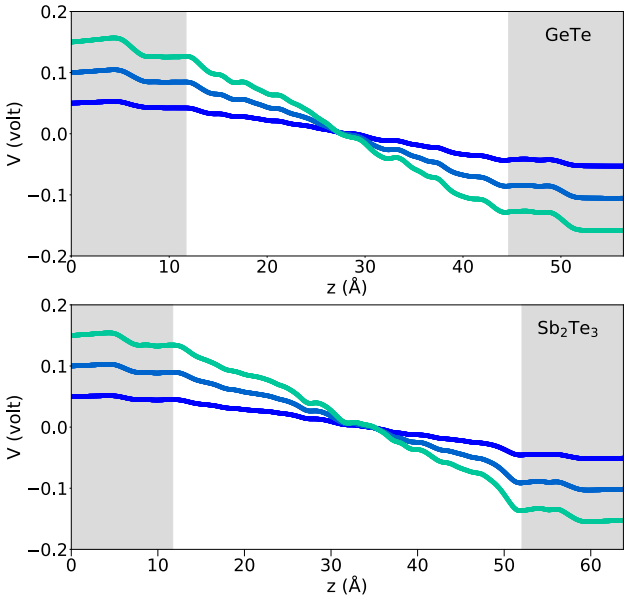

FIG. S4: Profile of the planar average of the electrostatic potential as a function of the position along the z direction in a representative Al/GeTe/Al model (upper panel) and Al/Sb_2Te_3/Al model (lower panel). The shaded area at the edges correspond to the two Al electrodes. Results for different bias between the two electrodes in the range 0.1-0.3 V are reported.

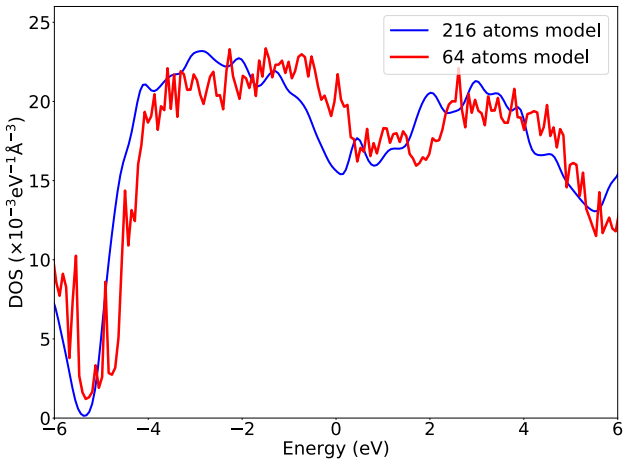

FIG. S5: Electronic density of states (DOS) close to the Fermi level (zero of energy) of a single snapshot of a 216-atom cell of liquid GeTe at 1150 K (see Ref. (1)) compared with the DOS projected on the central 51 atoms of the Al/GeTe/Al model at 1020 K (see Figs. 1-2 in the article). The DOS are computed with the code Siesta within the same framework used for the NEGF calculations (see article).

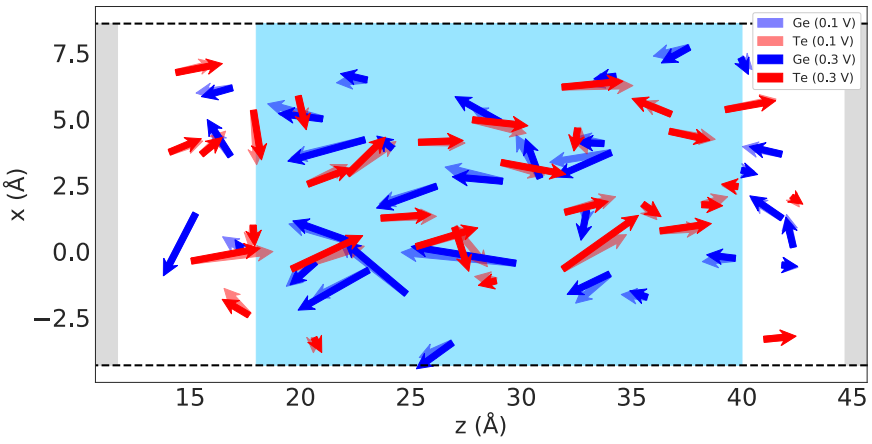

FIG. S6: Map of the electromigration forces taken as the different of the force at zero and finite bias on individual atoms. The projection of the forces in the xz plane is shown for a representative Al/GeTe/Al model at 0.1 V and 0.3 V bias between the electrodes. Only atoms in the central region where the planar averaged electric field is approximatively uniform are considered in the calculation of Z^* (shaded area).

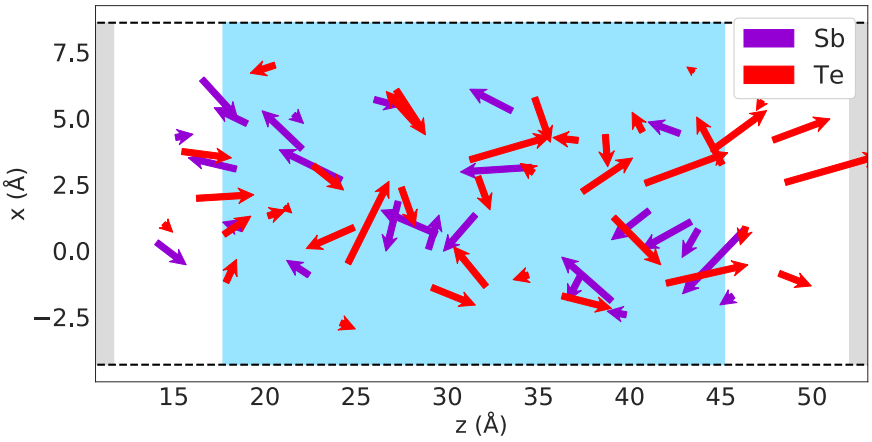

FIG. S7: Map of the electromigration forces taken as the different of the force at zero and finite bias on individual atoms. The projection of the forces in the xz plane is shown for a representative Al/Sb_2Te_3/Al model at 0.1 V bias between the electrodes. Only atoms in the central region where the planar averaged electric field is approximatively uniform are considered in the calculation of Z^* (shaded area).

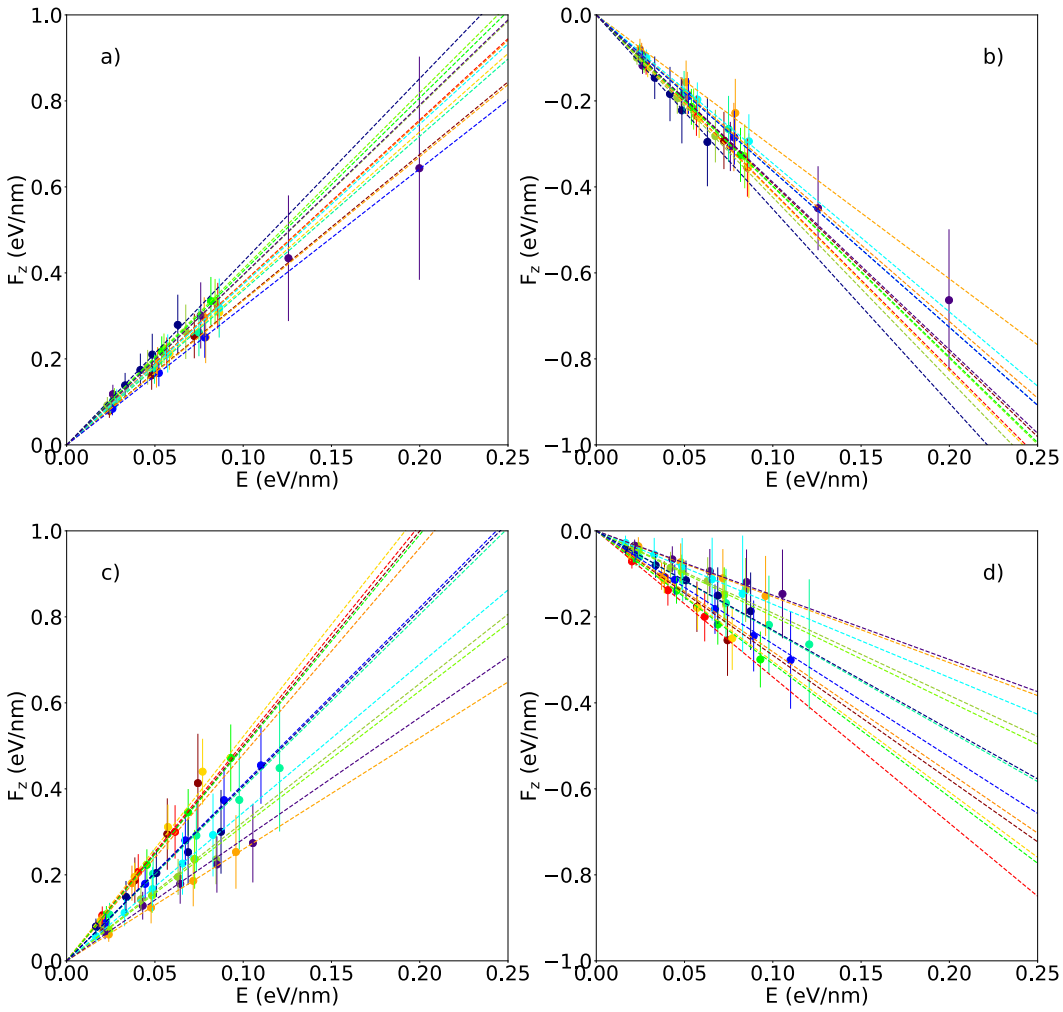

FIG. S8: Electromigration forces as a function of electric field for a) Ge atoms in GeTe, b) Te atoms in GeTe, c) Sb atoms in Sb_2Te_3 and d) Te atoms in Sb_2Te_3 for ten independent models. Each point is the result of the average over all atoms in the central region of a single model, i.e. for a single configuration of the liquid. The error bar is the spread in the values of the electromigration forces for the different atoms in a single model. Different colors correspond to different models.

References

(1) Sosso, G.; Caravati, S.; Behler, J.; Bernasconi, M. Neural network interatomic potential for the phase change material GeTe. *Phys. Rev. B* **2012**, *85*, 174103.

(2) Caravati, S.; Bernasconi, M.; Parrinello, M. First-principles study of liquid and amorphous Sb_2Te_3. *Phys. Rev. B* **2010**, *81*, 014201.